Numerical Methods and Data Analysis with Spreadsheets

I. Objective

To use spreadsheets to study the precision of several useful numerical methods (differentiation, integration, root solving) and to perform data analysis.

II. Introduction to Spreadsheets

One goal of Physics 232 is to point out the computational strengths and weaknesses of different software and calculation techniques. Though programming gives one complete control over how a calculation is done, there are many situations in which turning to a piece of software makes more sense. Therefore we should begin our introduction to spreadsheets by stating the types of calculations and number crunching that they do best.

- **Numerical algorithms that may be defined by an iterative formula:** There are many useful mathematical procedures where the value of the unknown depends on its value at a previous point. Examples include algorithms for *numerical differentiation, integration, root finding, and solving differential equations.* Formulas for several such methods are given in the Appendix.
- **Data analysis:** There are many useful ways to analyze experimental data using a spreadsheet. Of great value is the ability to easily import, manipulate, modify, and graph the data set.

In this lab we will apply spreadsheets to several of these procedures using the spreadsheet **MS Excel**. In class we will demonstrate several basic features of Excel that will assist you in completing today's exercises. These procedures are:

- Entering formulas and text
- Copying and pasting formulas
- Defining relative and absolute cell addresses
- Creating graphs

Today you will see how to use the capabilities of Excel to your advantage in numerical work and data analysis.

III. Exercises

A. Differentiation

Objective:	to compare derivative formulas of different orders
Where to begin:	start in MS Excel
What to do:	create a spreadsheet that studies the first two derivatives of the function $f = \sin(x)$ **at x = 1**
What to turn in to your instructor:	(1) graphs described below; (2) your comments on the results
What to put in log book:	the time you begin your work, problems, solutions, new commands, etc.

(1) **First derivative formulas:** We will compare the first derivative formulas given in the Appendix as a function of step size h at the point **x = 1** for the function $f(x) = \sin(x)$. Define the error $\Delta \equiv f'_{exact} - f'_{numerical}$. Create an appropriate spreadsheet that will allow you to study Δ as you change the step size h.

h	Δ for 3 pt formula	Δ for 5 pt formula
0.1		
0.01		
0.001		
0.0001		
0.00001		

(2) **Second derivative formulas:** Repeat the above exercise using the second derivative for both 3 point and 5 point formulas and now define $\Delta \equiv f''_{exact} - f''_{numerical}$.

Fill in the following table.

h	Δ for 3 pt formula	Δ for 5 pt formula
0.1		
0.01		
0.001		
0.0001		
0.00001		

(3) **Make log-log plot:** Use Excel's graphing functions to produce a log-log plot of Δ (on the y axis) versus h (on the x-axis) for both first and second derivatives comparing the 3 and 5 point formulas.

Comment on your results, especially why the error in the 5 point method increases below a certain step size (for a hint, get on Vincent and read **/home/physics/phys232/hint1**).

(4) **Save your work on your diskette:** Call your spreadsheet der1.xls.

B. Integration

Objective:	to compare the convergence of different integration formulas
Where to begin:	start in MS Excel
What to do:	create a spread sheet that performs the integral $\int_0^1 e^x dx$ using three methods
What to turn in to your instructor:	(1) graph described below; (2) your comments
What to put in log book:	the time you begin your work, problems, solutions, new commands, etc.

(1) **Compare three methods:** Create a spreadsheet for performing numerical integration that will compare the three methods given in the Appendix. You will calculate $\int_0^1 e^x dx$ for the Trapezoidal Rule, Simpson's Rule, and Bode's Rule using different numbers of intervals N. Define the error in the numerical calculation as $\Delta \equiv \int_{exact} - \int_{numerical}$ and use your spreadsheet to make the calculations necessary to fill in the table below.

N	$\Delta_{Trapezoidal}$	$\Delta_{Simpson}$	Δ_{Bode}
4			
8			
16			
32			
64			
128			

(2) **Make log-log plot:** Use Excel's graphing functions to produce a log-log plot of the calculation error Δ (on the y axis) versus N (on the x-axis) for each of the integration formulas.

Comment on the convergence of these different methods.

(3) **Save your work:** save your spreadsheet to your diskette calling it **int1.xls**.

C. Root Solving

Objective:	to study the convergence of the Secant Method of finding roots
Where to begin:	start in MS Excel
What to do:	create a spread sheet that determines the zeros of $f(x) = x^2 - 5$
What to turn in to your instructor:	a copy of your spreadsheet
What to put in log book:	the time you begin your work, problems, solutions, new commands, etc.

(1) **Root finding:** create a spreadsheet that applies the Secant Method given in the Appendix to solving for the roots of $f(x) = x^2 - 5$. Play around with the values of the first two points and see how quickly the method converges for very large initial values. Save your work on your disk in a file called **root1.xls**.

D. Data Analysis

Objective:	to study a nuclear magnetic resonance spectrum for hydrogen using techniques explored above
Where to begin:	FTP (to down-load), then go to MS Excel
What to do:	down-load the data file **/home/physics/phys232/nmr** from Vincent and create a spread sheet that performs the tasks below
What to turn in to your instructor:	(1) a copy of your graphs (no data please); (2) an estimate of the ratio R (defined below)
What to put in log book:	the time you begin your work, problems, solutions, new commands, etc.

(1) **Down-load NMR data:** use FTP to down-load the data file /home/physics/phys232/nmr from the Physics 232 locker to your PC. Copy the file to your A: drive and delete the file from the C: drive.

In Excel, use the **File** menu to locate the **Open** command, and open the file **nmr** on your **A:** drive. Read the text given above the data (you may wish to delete the text after reading it).

(2) **Plot the data:** use Excel's graphing functions to graph the data. Notice there are two peaks, one big and one small.

(3) **Separate the peaks:** find a function f_{small} that will fit the small peak. We will assume that the small peak may be modeled by a Gaussian function of the form

$$f_{small}(x) = Ae^{-\frac{(x-B)^2}{2C^2}}$$

Determine the values of A, B, and C that give a reasonable fit to the small peak. We will now assume that

$$f_{data}(x) = f_{small}(x) + f_{big}(x)$$

Use this relation to determine $f_{big}(x)$

(4) **Integrate under the peaks:** use one of the integration methods in the Appendix to determine the areas under the small and large peaks. What is the ratio of areas R of the large to small peak?

E. Access Maple

Before you leave, check to see if you can access **Maple** from your Vincent account. To do this, type **maple** at the Vincent prompt. If you cannot access Maple, let us know.

IV. Appendix: Formulas for Numerical Algorithms[1]

A. Notation

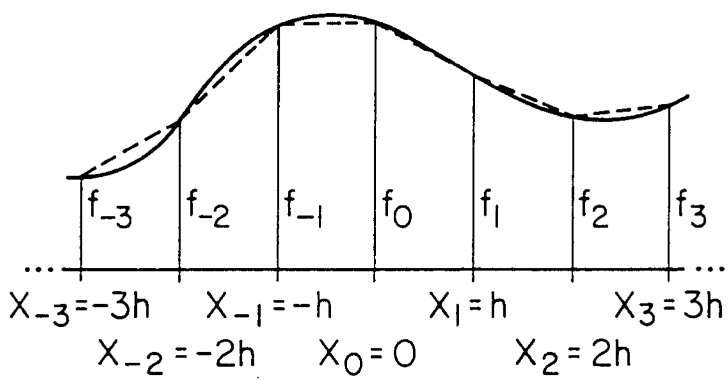
The following formulas are all based on the assumption that the function f(x) is defined on a number line of equally spaced coordinates. We define the following notation:

$$f_n \equiv f(x_n) \text{ where } x_n \equiv nh \ (n = 0, \pm 1, \pm 2, etc.)$$

The table below tells you how to think about this.

Think of ...	...as value of the function evaluated...
f_0	at the point of interest
f_1, f_{-1}	one lattice space to the right / left of f_0
f_2, f_{-2}	two lattice spaces to the right / left of f_0

The figure below illustrates this.



B. Differentiation

First Derivative Formulas			
Method Name	**Formula**	**Error**	**Reference**
3 point formula	$f' = \frac{1}{2h}[f_1 - f_{-1}]$	$O(h^2)$	Koonin p.5
5 point formula	$f' = \frac{1}{12h}[f_{-2} - 8f_{-1} + 8f_1 - f_2]$	$O(h^4)$	Koonin p.5
Second Derivative Formulas			
Method Name	**Formula**	**Error**	**Reference**
3 point formula	$f'' = \frac{1}{h^2}[f_1 - 2f_0 + f_{-1}]$	$O(h^2)$	Koonin p.5
5 point formula	$f'' = \frac{1}{12h^2}[-f_{-2} + 16f_{-1} - 30f_0 + 16f_1 - f_2]$	$O(h^4)$	Koonin p.6

[1] All of the differentiation and integration formulas are derived in the book *Computational Physics* by Steven Koonin which is on reserve in Parks Library. The formulas are obtained by writing the Taylor expansion of the function

$$f(x) = f_0 + xf' + \frac{x^2}{2!}f'' + \frac{x^3}{3!}f''' + \ldots$$

where all the derivatives are evaluated x = 0.

C. Integration

We will break up integrals over the range [a,b] into the smaller integrals (for Trapezoidal and Simpson's Rule)

$$\int_a^b f(x)dx = \int_a^{a+2h} f(x)dx + \int_{a+2h}^{a+4h} f(x)dx + \ldots + \int_{b-2h}^{b} f(x)dx$$

or (for Bode's Rule)

$$\int_a^b f(x)dx = \int_a^{a+4h} f(x)dx + \int_{a+4h}^{a+8h} f(x)dx + \ldots + \int_{b-4h}^{b} f(x)dx$$

and apply the formulas for the smaller integrals given below. Note that the interval length h is $h = \frac{b-a}{N}$ where N is the number of intervals. Note from the table that N must be chosen to be a multiple of 2 or 4 for the methods below.

Integration Formulas

Method Name	Formula	Error	N	Reference
Trapezoidal Rule	$\int_{-h}^{h} f(x)dx = \frac{h}{2}\left(f_{-1} + 2f_0 + f_1\right)$	$O(h^3)$	must be a multiple of 2	Koonin p.6
Simpson's Rule	$\int_{-h}^{h} f(x)dx = \frac{h}{3}[f_1 + 4f_0 + f_{-1}]$	$O(h^5)$	must be a multiple of 2	Koonin p.6
Bode's Rule	$\int_0^{4h} f(x)dx = \frac{2h}{45}[7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4]$	$O(h^7)$	must be a multiple of 4	Koonin p.8

D. Root Solving

Method Name	Recursion Formula	Reference
Secant Method	$x_{i+1} = x_i - f(x_i)\left(\frac{x_i - x_{i-1}}{f(x_i) - f(x_{i-1})}\right)$	Koonin p.12